ED-cPSD Documentation

Andre Adam, Guang Yang, Huazhen Fang, Xianglin Li

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Contents

Introduction

This document serves as reference and documentation for ED-cPSD, a software based on a novel algorithm of sequential erosion-dilation for continuous phase-size distribution (ED-cPSD) estimation. This document is segmented into a few different chapters which serve as reference for both users and contributors.

Chapter 1 is dedicated to get new users running the software and generating meaningful results immediately. Chapter 1 will walk new users through the installation process, basic GUI usage, running code de-coupled from the GUI, preparing inputs with ImageJ [1] and/or simple python scripts (OpenCV), expected outputs, and interpreting outputs.

Chapter 2 will first present an in-depth mathematical description to the algorithm working behind the scenes to calculate the continuous phase-size distribution (cPSD). This chapter also includes implementation details for both the standalone code and the GUI computational model. These implementation details are important for someone who is looking to contribute to and/or fork this project.

Chapter 3 presents several examples and case studies of the use of this software/algorithm. Each case study carries highlights quintessential aspects of the algorithm, such as discussions on how to interpret the output data given different inputs, comparisons with other cPSD and discrete phase-size distribution (dPSD) algorithms, and use cases in materials science and energy research.

Finally, chapter 4 has additional information, such as acknowledgments, code licensing information, and references.

Chapter 1

Quick-Start Guide

Chapter 2

Algorithm Details

2.1 Motivation

The interplay between different phases in heterogeneous materials [2] is of paramount importance in determining the bulk-scale properties of said materials. More specifically, in porous media, the interplay between the particle and pore spaces are critical in determining the transport properties, as has been thoroughly discussed in scattered studies[3, 4, 5, 6, 7, 8, 9].

Several software packages and algorithms already aim take aim at reconstructing, analyzing, and characterizing the morphology of such complex systems, such as MCRpy [10] and MATBOX [11]. On the other hand, there are different interpretations on the meaning and accuracy of physical descriptors.

One such property is the particle/pore/phase size distribution, which is often reported as just the average pore/particle diameter, D_{50}. This is obviously an issue, as there is often no definition of what consists a particle or a pore, much less a single determination of what "size" means without context (i.e. what is the size of an ellipsoid? The semi-major axis, the semi-minor axis, the average diameter, the length, or an average of all of those?).

In some materials, like carbon-based materials for battery electrodes or some types of sandstone can be observed under scanning electron microscopy (SEM) to be largely composed of small approximately spherical individual particles. In such cases, segmenting particles within the domain and assigning them sizes is feasible, in what is considered a discrete particle-size distribution (dPSD) algorithm.

While different dPSD algorithms have different approaches, the basic scheme is the same: each domain is segmented into particles, and each particle is labeled separately. Then, the morphology of each particle is quantified, and from there the averages can be obtained (i.e. PSD and D_{50}. More details and a brief compilation of such algorithms can be found in Usseglio-Viretta (2020) [12].

Another avenue for obtaining the PSD is via continuous pore-size distribution (cPSD) algorithms. This class of algorithms implies a continuous assessment of the size of each phase space. In other words, no segmentation is needed and there is a continuous measurement of phase-space morphology. This interpretation is more consistent when considering materials like stochastic aluminum foams [13], where both the aluminum and pore-space are continuous and amorphous, hence incompatible with dPSD.

Even in better structured materials like triply-periodic minimal surfaces (TPMS), the cPSD measurements of particles and pore size distributions are physically interpretable, representing the probability density of thickness distribution and pore-space minimum radius distribution, respectively. Or, in the aforementioned examples of carbon-based battery electrodes and sandstone, the pore-space is simply the interstitial space defined by the absence of solid particles, hence it is also continuous and amorphous. Approaching such cases with a dPSD algorithm can be tricky, as it can quickly lead to over-segmentation [12].

Furthermore, the cPSD class of algorithms more closely resemble mercury intrusion porosimetry [14] or nitrogen desorption porosimetry [15], which are experimental methods for determining pore-size distributions. Again, a brief review and further discussion can be found in Usseglio-Viretta (2020) [12].

On the other hand, the cPSD algorithms do have several downsides [12], including the necessity for data fitting, strong assumptions about particle shape (the spherical-particle assumption), the lack of information about the location and anisotropy of the related spaces, no mechanism for particle identification, requiring large representative volumes for accurate assessment, and often times underestimation of average phase sizes.

2.2 cPSD via Sequential Erosion-Dilation: ED-cPSD

The ED

Chapter 3

Case Studies

Chapter 4

Additional Information

4.1 Acknowledgments

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